

**User's Guide for CEMC\_SFU\_AGRO  
v1.2**

**The Combined Canadian Environmental  
Modelling Centre Water Quality Model and the  
Simon Fraser University Food Web Model**

**Version 1.2**

September 18, 2007

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## Introduction

The Canadian Environmental Modelling Centre's AGRO modeling system (AGRO) is a MicroSoft Excel® based application that combines a water quality model with a food web model to estimate risk to aquatic species from pesticide exposure in a user-defined water body. A major feature of this system is its capability to incorporate dynamic functionalities which allow the user to introduce changing environmental and emission conditions so that the fate and bioaccumulation results of numerous chemicals can easily and efficiently be compared.

The AGRO modeling system is written in Visual Basic and has an EXCEL® interface for parameter input and output display. This system can be run in dynamic mode which uses daily input of water, sediment, and pesticide from predicted daily mass loadings generated by US EPA Pesticide Root Zone Model, version 3.12 (PRZM3.12) (Suárez, 2006). [Note: AGRO can also be run in a steady-state mode]. Daily loading and emission values from PRZM3.12 are then used to generate predicted daily pesticide concentrations in the water column, benthic pore water and benthic sediment of the water body. From these concentrations, the food web model estimates bioaccumulation of pesticide in aquatic organisms.

The water quality model component of the AGRO modeling system is the Quantitative Water, Air, Sediment Interaction (QWASI) Fugacity model developed by Mackay et al. at the Canadian Environmental Modelling Centre (Mackay, Joy and Paterson (1983), Mackay, Paterson and Joy (1983), Mackay and Diamond (1989), Webster, Lian and Mackay (2005)). The QWASI model is based on a single receiving water body of user-defined size and depth with an active sediment layer. This model can be run in dynamic mode which involves daily input of water from field runoff, dissolved pesticide in field runoff, eroded sediment, pesticide sorbed to eroded sediment, pesticide emissions resulting from application drift and rainfall. These dynamic daily inputs are generated outside of the AGRO modeling system using the EPA PRZM3.12. The AGRO modeling system has built-in capability to import annual mass loading files output from PRZM3.12 and convert these values into the units and configurations needed by the QWASI Fugacity model.

The food web model in AGRO is based on the Bioaccumulation model developed by Frank A.P.C. at Simon Fraser University (Gobas, 2007). The Bioaccumulation model is a dynamic or time dependent interpretation of Arnot and Gobas [2004] bioaccumulation equation. This model is based on the assumption that the exchange of hydrophobic organic chemicals between the organism and its ambient environment can be described by a single equation for a large number of aquatic organisms. For each aquatic organism, this equation estimates bioaccumulation as a function of intake of pesticide via respiration and ingestion of prey, and outflow of pesticide via excretion, metabolism to a daughter product and respiratory exhalation.

## System Requirements

The AGRO modeling system is designed to run using MicroSoft Excel® 2003 with at least 10 MB of hard disk space.

## Computation Flow Overview

Using Visual Basic for Applications (VBA) as the programming language allows for the AGRO modeling system to function within the framework of EXCEL spreadsheets, thus facilitating the entry and viewing of both the input parameters and the display and analysis of the subsequent output. The following steps detail how to run the AGRO modeling system.

**To run the AGRO modeling system in dynamic mode:**

### Step 1 - Import Daily Mass Loading Data Generated by PRZM3.12 for use in the QWASI model.

Go to the **Get\_PRZM\_Files** Tab

Here is an example of a Get\_PRZM\_Files page:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	Collected Data for verification against textfiles						Get PRZM data	Start Year	1961	Location of PRZM Files	C:\project\071913F\AGRO PE5 interface\PE5-C1.D				
2	Field Area Ha	10						End Year	1964		Most recent year already loaded	1990			
3															
		Year	Month	Day	app rate kg/ha	app eff	pot drift	runoff depth cm/day	runoff flux (g/cm2/day)	ero soil loss tonnes/ha/ p/cm2/day	ero pest flux g/cm2/day	precip cm			
135		132	1961	5	12	1	0.99	5	0	0	0	0			
136		133	1961	5	13	0	0	0	0.122	1.72E-08	0.002343	1.019E-10	1.65		
137		134	1961	5	14	0	0	0	0	0	0	0	0		
138		135	1961	5	15	0	0	0	0	0	0	0	0		
139		136	1961	5	16	0	0	0	0	0	0	0	0		
140		137	1961	5	17	0	0	0	0	0	0	0	0		
141		138	1961	5	18	0	0	0	0	0	0	0	0		
142		139	1961	5	19	1	0.99	5	0	0	0	0	0		
143		140	1961	5	20	0	0	0	0	0	0	0	0		
144		141	1961	5	21	0	0	0	0	0	0	0	0		
145		142	1961	5	22	0	0	0	0	0	0	0	0		
146		143	1961	5	23	0	0	0	0	0	0	0	0		
147		144	1961	5	24	0	0	0	0	0	0	0	0		
148		145	1961	5	25	0	0	0	0	0	0	0	0		
149		146	1961	5	26	1	0.99	5	1.188	3.3E-07	0.08869	2.433E-09	3.71		
150		147	1961	5	27	0	0	0	0.4006	8.62E-08	0.0195	2.276E-10	1.47		
151		148	1961	5	28	0	0	0	0.2194	3.69E-08	0.007882	3.839E-11	1.14		
152		149	1961	5	29	0	0	0	0.0255	3.64E-09	0.00028	1.215E-12	0.61		
153		150	1961	5	30	0	0	0	0	0	0	0	0		
154		151	1961	5	31	0	0	0	0	0	0	0	0		
155		152	1961	6	1	0	0	0	0	0	0	0	0		
156		153	1961	6	2	1	0.99	5	0	0	0	0	0		
157		154	1961	6	3	0	0	0	0	0	0	0	0		
158		155	1961	6	4	0	0	0	0	0	0	0	0		
159		156	1961	6	5	0	0	0	0	0	0	0	0		
160		157	1961	6	6	0	0	0	0	0	0	0	0		
161		158	1961	6	7	0	0	0	0	0	0	0	0		
162		159	1961	6	8	0	0	0	0	0	0	0	0		
163		160	1961	6	9	0	0	0	0.9251	1.55E-07	0.05806	4.29E-10	2.24		

Click the “**Get PRZM data**” button located on cells Get\_PRZM\_Files!G(1:2)-Get\_PRZM\_Files!H(1:2). Clicking this executes a Visual Basic macro which

allows the user to choose the location of the PRZM3.12 P2E-c1.D\* mass loading files. Click on any of the P2E-C1.D\* files and then “Open” to begin the import of the mass loading values and to store them in this tab. This macro also converts the data into the units and variables compatible with the QWASI model. These converted values are stored in the **PRZMforInput** tab.

Table 1 below summarizes the conversion of massing loading values in the P2E-C1.D\* files into the values stored in the **PRZMforInput** tab.

**Table 1: Summary of daily input values for AGRO model derived from PRZM output**

<i>Parameter</i>	Description
<i>Simday</i>	assigned to evaluate and loop through the total number of days of data provided by PRZM
<i>Year Month Day</i>	from PRZM
<i>E to Pond kg/y</i>	this is the 5% spray drift from PRZM expressed as kg/y
<i>Inflow-W Conc ng/L</i>	from PRZM expressed in ng/L
<i>Inflow-P Conc ng/L</i>	from PRZM expressed in ng/L
<i>Bulk Inflow Conc ng/L</i>	uses Inflow-W Conc and Inflow-P Conc with the respective volume fractions to calculate a bulk water concentration of chemical
<i>Water Inflow rate m<sup>3</sup>/h</i>	Standard rate defined on Environment worksheet + PRZM runoff
<i>Particulate Inflow rate m<sup>3</sup>/h</i>	Standard rate derived from Environment worksheet +PRZM erosion rate
<i>Inflow-P concentration</i>	derived Inflow and Particulate inflow rates
<i>VF-W Inflow</i>	Volume Fraction of water in the inflow
<i>VF-P Inflow</i>	Volume Fraction of particulate in the inflow
<i>rain rate m<sup>3</sup>/h</i>	converted from cm/day in PRZM to m <sup>3</sup> /h

The AGRO modeling system also contains a blank worksheet with tab entitled, **PRZM-workarea**. This worksheet is used by the AGRO Visual Basic module to store internal variable values during processing. It is always cleared at the end of each instance of retrieval of PRZM files.

## Step 2 – Enter or Select Chemical Input Parameters

Go to the **Chemical** tab

The chemical parameters are defined here. A “database” of chemical parameters is listed in columns Chemical!Q through Chemical!AK.

Here is an example of columns Chemical!Q through Chemical!AK in the **Chemical** Tab:

	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AD	AE	AF	AG	AH	AI	AJ	AK
				ChemName	Type	Property Temperature	Molecular Mass (g/mol)	Melting Point C	Solubility (g/m3)	Vapour Pressure (Pa)											
1	Chemical	1	#																		
2				1 Test Chemical	1	17	345.6	125	1.79	1.24E-08		5.1		240	960						
3				2 Food Web Sensitivity Analysis	1	17	506.4	300	1	1.00E-04		5.1		720	720						
4				3 Modeling for EFED Report	1	17	506.4	300	1.79	1.24E-08		5.1		96	9072						
5																					
6																					
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34																					

More chemicals can be added to this database or existing chemicals can be modified by entering data into the appropriate columns in the “tan” shaded areas. The names of the newly added chemicals will appear in the list-box entitled “Select a Chemical” in columns Chemical!D-Chemical!F of this tab.

To enter a new chemical with Type I partitioning into the chemical database, enter the following chemical information into the first available empty row:

**Table 2: Chemical Parameters for Type I Partitioning Simulations**

Column	Parameter	Units	Notes
Chemical!Q	Chemical Identifier	---	The row number plus 1. This will be used as the chemical number identifier.
Chemical!R	Chemical Name	---	Name of chemical of interest
Chemical!S	Chemical Type	---	1 for Type I partitioning and 2 for Type II partitioning. For regulatory modeling, Type I partitioning is employed.
Chemical!T	Property Temperature	°C	Default 17°C
Chemical!U	Chemical Molecular Mass	g/mol	Molecular weight of chemical
Chemical!V	Chemical Melting Point °	°C	
Chemical!W	Solubility	g/m <sup>3</sup>	Water solubility of chemical. Equivalent units are kg/L.
Chemical!X	Chemical Vapor Pressure	Pa	
Chemical!Z	Log K <sub>OW</sub>	(mg/L)/(mg/L)	Log 10 of the Octanol-Water Partition Coefficient, K <sub>OW</sub>
Chemical!AD	Chemical Half-life in Water	days	Aqueous aerobic half-life
Chemical!AE	Chemical Half-life in Sediment	days	Aqueous anaerobic half-life

For Type I chemicals, Columns Chemical!AG-Chemical!AK are left blank. For Type II chemicals (those with little or no volatility) only the Molar Mass, Property Temperature, Degradation Half-lives and partition coefficients defined in Chemical!AG:Chemical!AK (with appropriate units) are used. Please see Mackay (2001) for more information on modelling Type I and Type II chemicals.

**Table 3: Chemical Parameters for Type I Partitioning Simulations**

Column	Parameter	Units	Notes
Chemical!Q	Chemical Identifier	---	The row number plus 1. This will be used as the chemical number identifier.
Chemical!R	Chemical Name	---	Name of chemical of interest
Chemical!S	Chemical Type	---	1 for Type I partitioning and 2 for Type II partitioning.
Chemical!T	Property Temperature	°C	Default 17°C
Chemical!U	Chemical Molecular Mass	g/mol	Molecular weight of chemical
Chemical!AD	Chemical Half-life in Water	days	Aqueous aerobic half-life
Chemical!AE	Chemical Half-life in Sediment	days	Aqueous anaerobic half-life
Chemical!AG	Air/Water Partition Coefficient, $K_{AW}$	dimensionless	
Chemical!AH	Aerosol/Water $K_{QW}$	dimensionless	
Chemical!AI	Sediment-Water	L/kg	
Chemical!AJ	Suspended Sediment-Water	L/kg	
Chemical!AK	Resuspended Sediment-Water	L/kg	

Now, go to the list-box “Select a Chemical” in columns Chemical!D-Chemical!F. Highlight the chemical of interest and click the “OK” button. This will cause the appropriate values of the selected chemical to appear in column Chemical!B where the user can easily review them and where the model actually reads the values used in the upcoming simulation. (If the user wishes to make temporary changes to a chemical data, these can be made directly in column Chemical!B without affecting the original values in the database, although these value will be overwritten each time the “OK” button is clicked)



Here is an example of columns Chemical!A through Chemical!N (Rows 1-21) in the **Chemical** tab:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	<b>Chemical properties</b>													
2	Chemical Name	testazole												
3	Chemical Type	1												
4	Property Temperature C	17												
5	Molecular Mass (g/mol)	345.6												
6	Melting Point (C)	125												
7	Solubility (g/m <sup>3</sup> )	1.79												
8	Vapour Pressure (Pa)	1.23989E-08												
9	<b>Partitioning</b>													
10	logK <sub>OW</sub>	5.1												
11	logK <sub>AW</sub>													
12	logK <sub>OA</sub>													
13	<b>Degradation half-lives (h)</b>													
14	Water	240												
15	Sediment	960												
16	<b>Type II partitioning</b>													
17	Air-Water K <sub>AW</sub> (dimensionless)													
18	Aerosol-Water K <sub>OW</sub> (dimensionless)													
19	Sediment-Water (L/kg)													
20	Suspended Sediment-Water (L/kg)													
21	Resuspended Sediment-Water (L/kg)													

Select a Chemical:

testazole

Food Web Sensitivity Analysis

Modeling for EFED Report

OK

### Step 3 – Enter or Select Environment Input Parameters

Go to the **Environment** tab

The environment scenario parameters are defined here. A “database” of environmental scenarios is listed in columns Environment!O through Environment!AW. The environmental parameters listed here are those required to run the QWASI 3.10 model.

The user may add environmental scenarios to this database by entering necessary information into the columns Environment!O through Environment!AW. The names of the newly added environments will appear in the list-box entitled “Select an Environment” in this tab.

Here is an example of columns Chemical!O through Chemical!AA of the environmental database in the **Environment** tab. Columns Environment!S through Environment!V refer to dimensions of the water body. Columns Environment!W through Environment!AA refer to the concentration of particle solids in the various bulk media. The “tan” cells indicate that the user may input data in these cells.

	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	
	Selected Environment	2	Environmental Properties	Name	Dimensions	Water_Surface_Area	Water_Volume	Sediment	Concentration of Solids	Aerosol_Particles	Particles_Inflow	Particles_Water_Column	Volume_Fraction_Particles_Surface	Der Sol (kg)
1														
2			1	Sensitivity Analysis		10000	20000	0.05		30	2	30	0.5	
3			2	Modeling for EFED Report		10000	20000	0.01		30	2	30	0.5	
4														
5														
6														
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23														

Splitting the screen after column Environment!R and scrolling right, displays columns Environment!AB through Environment!AE which pertain to the density of solids in the various bulk media. Columns Environment!AF through Environment!AJ which pertain to the fraction of organic carbon in the various bulk media.

	O	P	Q	R	AB	AC	AD	AE	AF	AG	AH	AI	AJ	
	Selected Environment	2	Environmental Properties	Name	Density of Solids (kg/m <sup>3</sup> )	Density_Particles_Water	Density_Sediment_Particles	Density_Aerosol_Particles	Organic Carbon Fraction of Solids	Fraction_Organic_Carbon_Water	Fraction_Organic_Carbon_Sediment	Fraction_Organic_Carbon_Inflow	Fraction_Organic_Carbon_Resuspended	Flow
1														
2				1 Sensitivity Analysis		2400	2400	1500		0.067	0.014	0.067	0.014	
3				2 Modeling for EFED Report		2400	2400	1500		0.067	0.04	0.067	0.04	
4														
5														
6														
7														
8														
9														
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23														

Splitting the screen after column Environment!R and further scrolling right, displays columns Environment!AK through Environment!AP which pertain to the flow rates for the water and sediment in various bulk media.

	O	P	Q	R	AK	AL	AM	AN	AO	AP	Formula Bar	AS	
	Selected Environment	2	Environmental Properties	Name	Flows	River_Water_Inflow	Water_Outflow_Rate	Deposition_Rate	Burial_Rate_Solids	Resuspension_Rate	Mass Transfer Coefficients	Aerosol_Dry_Deposition_Ratio	Scavenging_Ratio
1													
2				1 Sensitivity Analysis		5	5	80	40	40		10	200000
3				2 Modeling for EFED Report		5	5	50	10	40		10	200000
4													
5													
6													
7													
8													
9													
10													
11													
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Splitting the screen after column Environment!R and further scrolling right, displays columns Environment!AQ through Environment!AW which pertain to the mass transfer coefficients characterizing intermedia transport .

	O	P	Q	R	AQ	AR	AS	AT	AU	AV	AW	AX	AY
	Selected Environment	2	Environmental Properties	Name	Mass Transfer Coefficients	Aerosol_Dry_Deposition_Ratio	Scavenging_Ratio	Rain_Rate	Vol_Mass_Transf_Coeff_Air	Vol_Mass_Transf_Coeff_Water	Sediment-Water_Diffusion		
1													
2				1 Sensitivity Analysis		10	200000	1	0.5	0.005	0.0008		
3				2 Modeling for EFED Report		10	200000	1	1	0.01	0.0004		
4													
5													
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Here is a summary of the input Parameters in the **Environment** Tab:

**Table 4: Input Parameters in the Environment Tab**

*Note: Default values for EPA generic pond scenario are listed in notes column.*

Column	Parameter	Units	Notes
Environment!O	<b>“Dimensions”</b>	---	Label for columns associated with dimensions of the water body
Environment!P	Selected Environment Identifier	---	Numeric identifier of environmental scenario highlighted in the “Select an Environment” list-box. Automatically changes with change in highlighted selection.
Environment!Q	Environmental Properties Scenario Identifier	---	User-supplied numeric identifier of environmental scenario of interest
Environment!R	Name of Environmental Scenario	---	Name given to the environmental scenario
Environment!T	Water_Surface_Area	m <sup>2</sup>	Surface area of water body Default value: 10,000
Environment!U	Water_Volume	m <sup>3</sup>	Volume of water body Default value: 20,000
Environment!V	Sediment	m	Depth of sediment in benthic layer. Default value: 0.05
Environment!W	<b>“Concentration of Solids”</b>	---	Label for columns associated with concentration of solid particles in various bulk media
Environment!X	Aerosol_Particles	ug/m <sup>3</sup>	Concentration of solid particles in air bulk media. Default value: 30
Environment!Y	Particles_Inflow	mg/L	Concentration of solid particles in inflow water bulk media. Default Value: 2
Environment!Z	Particles_Water_Column	mg/L	Concentration of suspended sediment in water column. Default value: 30
Environment!AA	Volume_Fraction_Particles_Surface	m <sup>3</sup> /m <sup>3</sup>	Volume fraction of sediment particles in benthic. Default value: 0.5

Column	Parameter	Units	Notes
Environment!AB	<b>“Density of Solids”</b>		Label for columns associated with density of solid particles in various bulk media
Environment!AC	Density_Particles_Water	kg/m <sup>3</sup>	Density of solid particles in water column bulk media. Default value: 2400
Environment!AD	Density_Sediment_Particles	kg/m <sup>3</sup>	Density of solid particles in benthic sediment bulk media. Default value: 2400
Environment!AE	Density_Aerosol_Particles	kg/m <sup>3</sup>	Density of solids particles in air bulk media. Default value: 1500
Environment!AF	<b>“Organic Carbon Fraction of Solids”</b>		Label for columns associated with organic carbon fraction in various bulk media
Environment!AG	Fraction_OC_Water	---	Fraction of organic carbon in water column bulk media. Default value: 0.067
Environment!AH	Fraction_OC_Sediment	---	Fraction of organic carbon in benthic sediment bulk media Default value: 0.014
Environment!AI	Fraction_OC_Inflow	---	Fraction of organic carbon in inflow water bulk media Default value: 0.067
Environment!AJ	Fraction_OC_Resuspended	---	Fraction of organic carbon in resuspended sediment. Default value: 0.014

Column	Parameter	Units	Notes
Environment!AK	<b>“Flows”</b>		Label for columns associated with flow rates in various bulk media
Environment!AL	River_Water_Inflow	m <sup>3</sup> /h	Flow rate of inflow water into water body. Default value: 5
Environment!AM	Water_Outflow_Rate	m <sup>3</sup> /h	Flow rate of outflow water out of the water body. Default value: 5
Environment!AN	Deposition_Rate	g/m <sup>2</sup>	Deposition rate of solid particles to benthic sediment. Default value: 80
Environment!AO	Burial_Rate_Solids	g/m <sup>2</sup>	Burial rate of solid particles in benthic sediment. Default value: 40
Environment!AP	Resuspension_Rate	g/m <sup>2</sup>	Resuspension rate of solid particles out of the benthic and back into the water column. Default value: 40
Environment!AQ	<b>“Mass Transfer Coefficients”</b>		Label for columns associated with Mass transfer Coefficients between various bulk media
Environment!AR	Aerosol_Dry_Deposition	m/h	Deposition rate of dry particles out of air into water body. Default value: 10
Environment!AS	Scavenging_Ratio	Volume of air/Volume of Rain	Scavenging Ratio of air to rain Default value: 20,000
Environment!AT	Rain_Rate	m/year	Rainfall rate in meters per year. Default value: 1
Environment!AU	Vol_Mass_Trans_Coeff_Air	m/h	Volatilization rate – air side Default value: 1
Environment!AV	Vol_Mass_Transfer_Coeff_Water	m/h	Volatilization rate – water to air Default value: 0.01
Environment!AW	Sediment-Water-Diffusion	m/h	Diffusion rate between benthic sediment and water column. Default value: 0.0004

Now, go to the list-box “Select an Environment” in columns Environment!E-Chemical!G. Highlight the environment of interest and click the “OK” button. This will cause the appropriate values of the selected environment to appear in column Environment!B where the user can easily review them and where the model actually reads the values used in the upcoming simulation. (If the user wishes to make temporary changes to a chemical data, these can be made directly in column Environment!B without affecting the original values in the database, although these value will be overwritten each time the “OK” button is clicked)

Here is an example of columns Environment!A through Chemical!N (Rows 1-33) in the **Environment** tab:

The screenshot displays the PRZM model interface, specifically the 'Environment' tab. The main window shows a list of parameters organized into sections: Environmental Properties, Dimensions, Concentration of Solids, Density of Solids, Organic Carbon Fraction of Solids, Flows, and Mass Transfer Coefficients. A 'Select an Environment' dialog box is open, allowing the user to choose an environment from a list. The 'OK' button is visible at the bottom of the dialog. The background shows the PRZM model's file structure, including folders for AGRO, Chemical, Environment, and various output files.

Row	Parameter	Value	
1	<b>Environmental Properties</b>		
2	<b>Name</b>	<b>Modeling for EFED Report</b>	
3	<b>Dimensions</b>		
4	Water Surface Area (m <sup>2</sup> )	10000	
5	Water Volume (m <sup>3</sup> )	20000	
6	Sediment Active Layer Depth (m)	0.01	
7	<b>Concentration of Solids</b>		
8	Aerosol Particles (µg/m <sup>3</sup> )	30	
9	Inflow Particles (mg/L)	2	
10	Suspended Sediment (mg/L)	30	
11	Sediment Particles (m <sup>3</sup> /m <sup>3</sup> )	0.5	
12	<b>Density of Solids (kg/m<sup>3</sup>)</b>		
13	in Water	2400	
14	in Sediment	2400	
15	in Aerosols	1500	
16	<b>Organic Carbon Fraction of Solids</b>		
17	in Water	0.087	
18	in Sediment	0.04	
19	in Inflow	0.087	
20	in Resuspended Sediment	0.04	
21	<b>Flows</b>		
22	River water inflow (m <sup>3</sup> /h)	5	
23	Water outflow (m <sup>3</sup> /h)	5	
24	Deposition rate of solids to sediment (g/m <sup>2</sup> /day)	50	
25	Burial Rate of Solids (g/m <sup>2</sup> /day)	10	
26	Resuspension Rate of Solids (g/m <sup>2</sup> /day)	40	
27	<b>Mass Transfer Coefficients</b>		
28	Aerosol Dry Deposition (m/h)	10	
29	Scavenging Ratio (vol air/vol rain)	200000	
30	Rain Rate (m/h)	1	
31	Volatilization (air side) (m/h)	1	
32	Volatilization (water side) (m/h)	0.01	
33	Sediment-Water diffusion (m/h)	0.0004	



## Step 4 – Confirm the Emissions Parameters

Go to the **Emissions** tab

Here is what the Emissions tab page should look like when dynamic emission scenario is selected:

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1																
2	Emission Scenario:	Dynamic from PRZM													Emission Type	2
3																
4	Emission Type:															
5	<input type="radio"/> Constant, average annual emission (kg/Ha/year), input below															
6	<input checked="" type="radio"/> Defined daily emissions (kg/Ha/day), input from PRZM															
7																
8	Steady state type emission (kg/Ha/year)	1.1208		Field Area (Ha)	10											
9	Spray drift pulse kg/year (5% of annual emission)	0.5604														
10																
11	Ambient Concentration in Air (ug/m³)	0														
12	Ambient Concentration in Inflow Water (ng/L)	0														
13																
14																
15																
16																
17																
18																
19																
20																
21																
22																
23																
24																
25																
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27																
28																
29																
30																
31																
32																
33																
34																

On the **Emissions** tab, there are two options. By clicking on either radio button under the heading “Emission Type” the user may choose one of two scenarios. The first option is used for steady-state calculations or for dynamic ones requiring that there be constant emission of chemical over the duration of the model run. The second option is to use the PRZM-defined inputs imported to **PRZMforInput** and **GetPRZMFiles** tabs.

### Dynamic Emissions

To use the PRZM-defined inputs and parameters, make sure that the “Defined daily emissions (kg/Ha/day), input from PRZM” is selected so that the Emission Type in cell Emissions!P2 is set to 2. Cell Emissions!B2 should say “Dynamic from PRZM” and the cells Emissions!A8:Emissions!E12 appear as though “grayed-out”. The above set-up with “Defined daily emissions” selected activates the dynamic mode execution of the model where daily values are read from the **PRZMforInput** tab.

The internal model code automatically navigates through the **PRZMforInput** daily values until it reaches the first non-zero emissions occurrence in PRZMforInput!E column at which time the model iterations begin.

### **Constant Emissions**

If the “Constant Emission, average annual emission (kg/Ha/yr), input below” radio button is selected, the cells Emissions!A8:Emissions!E12 appear with a white background, except cells Emissions!B8, B11 and B12 which are “tan” in colour, indicating that they are user defined inputs. The model reads in the value for calculated direct inputs from spray drift to the pond from cell Emissions!B9. Note that the value of 5% of the application rate to 1 Ha is used to estimate the net input of chemical to the pond from all inputs. This is based on the US-EPA EXAMS model treatment of spray drift inputs to an agricultural pond.

The user may choose to enter any ambient air concentration of chemical in Emissions!B11 or inflow water concentration. Inflow water can be in the form of inflow derived from any source (inflow from another body of water, from groundwater or from runoff water), as long as the corresponding flow for this concentration is quantified on the Environment worksheet. The net annual input of chemical to the pond is derived using:

$$\text{Conc inflow ng/L} * \text{kg}/1 \times 10^{12} \text{ ng} * 1000 \text{ L/m}^3 * \text{Inflow rate m}^3/\text{h} * 8760 \text{ h/yr}$$

The result (kg/yr) inflow of chemical is added to the kg/yr estimate of direct emission to the pond via spray drift for a total chemical input rate.

## Step 5 – Review the FWModel tab

Go to the **FWModel** tab. This tab contains the chemical and ecosystem parameter values used by the Gobas Bioaccumulation model. Review the assigned input values.

Usually, the user will not make any revisions to this tab since the Environmental Fate Parameters on this worksheet are mostly calculated based on values entered in the **Environment and Chemical** tabs and the Food Web Bioaccumulation Model values are the recommended values for the embedded organism foodweb.

**Note: There is no database summarizing several possible foodwebs, so any changes made are permanent and it is suggested that an original version of the file be maintained at all times to preserve the original information.**

Columns FWModel!A through FWModel!G summarize the Chemical and Environmental Fate input parameters from the QWASI water quality model.

For columns FWModel!A through FWModel!G, rows 4 – 10, the chemical parameters required by the Bioaccumulation model are automatically summarized based on input values entered in the **Chemical** tab.

An example of columns FWModel!A through FWModel!G, rows 4 – 10 looks like:

	A	B	C	D	E	F
1	Environmental Fate Model					
2						
3	Model Input Parameters					
4	Chemical-Specific Properties	Symbol	Value	Action	Alternative Value	
5	Molecular Weight	MolW	345.6	Enter on Chemical Tab		
6	Henry's Law Constant (Pa.m3/mol)	H	2.39E-06	Calculated from Chemical Tab		
7	log Kow of the chemical	log Kow	5.1	Enter on Chemical Tab		
8	chemical half life in water (days)	hlw	10	Enter on Chemical Tab		
9	chemical half life in sediment (days)	hls	40	Enter on Chemical Tab		
10	log transformed organic carbon-water partition coefficient	log Koc	4.644068044	Calculated from Chemical Tab	original 0.35 Kow	
11						

For columns FWModel!A through FWModel!G, rows 12 – 31, the chemical parameters required by the Bioaccumulation model are automatically summarized based on input values entered in the **Environment** tab.

The following additional environmental input parameters along with their recommended values are required by the Bioaccumulation model:

**Table 5: Additional Environmental Input parameters in FWModel**

Input Parameter	Recommended Value
Dissolved oxygen saturation (%)	90%
Disequilibrium factor POC (unitless)	1
Disequilibrium factor DOC (unitless)	1
POC-octanol proportionality constant (unitless)	0.35
DOC-octanol proportionality constant (unitless)	0.08
pH of water	7
water temperature (degC)	17
Sediment OC octanol proportionality constant (unitless)	0.35
initial chemical mass in water (g)	0
initial chemical mass in sediment (g)	0

An example of columns FWModel!A through FWModel!G, rows 4 – 10 looks like:

	A	B	C	D	E	F	G
12	<b>System-Specific Characteristics</b>						
13	water body surface area (m <sup>2</sup> )	Saw	1.00E+04	Enter on Environment Tab			
14	sediment surface area (m <sup>2</sup> )	Sas	1.00E+04	Equal to Water Surface Area			
15	average water depth (m)	Dw	2	Calculated from Environment Tab			
16	depth of active sediment layer (m)	Ds	0.01	Enter on Environment Tab			
17	water in- and out-flow (L/day)	F	1.20E+05	Calculated from Environment Tab	4m <sup>3</sup> /h		
18	Concentration of particles in water (kg/L)	Cpw	3.00E-05	Calculated from Environment Tab		30mg/L	
19	Concentration of DOC in water (kg/L)	Cdoc	2.01E-06	Calculated from Environment Tab			
20	concentration of solids in sediment (kg/L)	Css	1.20E+00	Calculated from Environment Tab			
21	density of suspended solids (kg/L)	dpw	2.40E+00	Calculated from Environment Tab			
22	density of sediment solids (kg/L)	dss	2.40E+00	Calculated from Environment Tab			
23	organic carbon content of suspended solids (unitless)	Ocpw	6.70E-02	Enter on Environment Tab			
24	organic carbon content of bottom sediment (unitless)	Ocss	4.00E-02	Enter on Environment Tab			
25	density of organic carbon (kg/L)	dcc	1.00E+00	Enter			
26	water-side evaporation mass transfer coefficient (m/day)	vev	2.40E-01	Calculated from Environment Tab	0.01m/h		
27	air-side evaporation mass transfer coefficient (m/day)	vea	2.40E+01	Calculated from Environment Tab	1m/h		
28	water-to-sediment diffusion mass transfer coefficient (m/day)	vd	9.60E-03	Calculated from Environment Tab	0.0004m/h		
29	solids settling rate (g/m <sup>2</sup> /day)	vss	50	Enter on Environment Tab			
30	sediment burial mass transfer coefficient (g/m <sup>2</sup> /day)	vb	10	Enter on Environment Tab			
31	sediment resuspension rate (g/m <sup>2</sup> /day)	vsr	40	Enter on Environment Tab			
32	dissolved oxygen saturation (%)	S	90%	Enter		Lake Ontario	
33	Disequilibrium factor POC (unitless)	Dpoc	1	Enter			
34	Disequilibrium factor DOC (unitless)	Ddoc	1	Enter			
35	POC-octanol proportionality constant (unitless)	apoc	0.35	Enter		Lake Ontario	
36	DOC-octanol proportionality constant (unitless)	adoc	0.08	Enter		Lake Ontario	
37	pH of water	pH	7	Enter			
38	water temperature (degC)	Tw	17	Enter			
39	Sediment OC octanol proportionality constant (unitless)	asoc	0.35	Enter			

An example of columns FWModel!A through FWModel!G, rows 41 – 65 looks like:

	A	B	C	D	E	F	G
41	<b>Simulation Parameters</b>						
42	Time Increment (hours)	dt	3	From AGRO tab			
43	total external loading (g/day)	L	1.535342466	From Emissions tab			
44							
45	<b>Initial Enviromental Conditions</b>						
46	initial chemical mass in water (g)	Mwi	0	Enter			
47	initial chemical mass in sediment (g)	Msi	0	Enter			
48							
49							
50	<b>Rate Constants</b>						
51	outflow (/day)	ko	6.00E-03	Calculated	0.066352599	0.0242187	
52	volatilization (/day)	kv	6.18E-09	Calculated	6.83193E-08	2.4937E-08	
53	overall water-to-sediment transport (/day)	kws	7.11E-02	Calculated	0.786359071	0.28702106	
54	overall sediment-to-water transport (/day)	ksw	2.12E-03	Calculated	0.08390456	0.03062516	
55	solids settling (/day)	kws1	6.68E-02	Calculated	0.738339894	0.26949406	
56	water-to-sediment diffusion (/day)	kws2	4.34E-03	Calculated	0.048019177	0.017527	
57	solids resuspension (/day)	ksw1	1.67E-03	Calculated	0.06594502	0.02406993	
58	sediment-to-water diffusion (/day)	ksw2	4.54E-04	Calculated	0.01795954	0.00655523	
59	burial (/day)	kB	4.16E-04	Calculated	0.016486255	0.00601748	
60	degradation in water (/day)	kwr	0.069314718	Calculated	0.766535287	0.27978538	
61	degradation in sediment (/day)	ksr	0.01732868	Calculated	0.685968256	0.25037841	
62							
63							
64							
65							

An example of columns FWModel!A through FWModel!G, rows 66 – 87 looks like:

	A	B	C	D	E	F	G
65							
66	<b>Calculated Parameters</b>						
67	volatilization mass transfer coefficient (m/day)	ve	1.36584E-08	Calculated			
68	partition coefficient of suspended particles in the water	Kpw	2952.180091	Calculated			
69	partition coefficient of bottom sediment particles	Kps	1762.495577	Calculated			
70	air-water partition coefficient (unitless)	Kaw	5.69E-10	Calculated			
71	temperature dependence of Henry law constant (H)	ln H(Tw)	-1.35E+01	Calculated			
72	fraction of freely dissolved chemical in water (unitless)	fDW	90.46%	Calculated			
73	fraction of freely dissolved chemical in sediment (unitless)	fDS	0.05%	Calculated			
74	settling of sediment solids flux (kg/day)	SetFlux	2.00E+01	Calculated			
75	burial flux of sediment solids (kg/day)	BurFlux	5.00E+03	Calculated			
76	temperature dependence of Henry law constant (H)	H(Tw)	1.37213E-06	Calculated			
77	sediment solids mass balance and resuspension flux (kg/day)	ResFlux	-4977.60751	Calculated			
78	water volume of lake (m³)	Vw	2.00E+04	Calculated			
79	sediment volume (m³)	Vs	1.00E+02	Calculated			
80	Octanol-water partition coefficient (unitless)	Kow	1.26E+05	Calculated			
81	organic carbon-water partition coefficientn (L/Kg)	Koc	4.41E+04	Calculated			
82	Bioavailable solute fraction (unitless)	Φ	0.901868644	Calculated			
83	Concentration of particulate organic carbon (kg/L)	Xpoc	0.00000201	Calculated			
84	Concentration of dissolved organic carbon (kg/L)	Xdoc	2.01E-06	Calculated			
85	volume of sediment solids (kg)	Vss	1.20E+05	Calculated			
86	volume of sediment solids (L)	Vssl	5.00E+04	Calculated			
87	volume of pore water in sediment (L)	Vws	5.00E+04	Calculated			
88							

An example of columns FWModel!A through FWModel!G, rows 66 – 87 looks like:

	A	B	C	D	E	F	G
89	<b>Steady-state Mass Balance</b>						
90	total mass of chemical into water (g)	dMw/dt	1.62E+00	Calculated			
91	total mass of chemical out of water (g)	dMw/dt	1.62E+00	Calculated			
92	total mass of chemical into sediment (g)	dMs/dt	7.86E-01	Calculated			
93	total mass of chemical out of sediment (g)	dMs/dt	7.86E-01	Calculated			
94							
95							
96	<b>Steady State Evaluation</b>						
97	total mass of chemical in water (g)	Mw	11.06	Calculated	35.77		
98	total mass of chemical in sediment (g)	Ms	39.59	Calculated	458.33		
99							
100	<b>Concentrations</b>						
101	freely dissolved concentration of chemical in water (g/L)	Cwdo	4.9968E-07	Calculated	1.6203E-09		
102	concentration of chemical in water (g/L)	Cw	5.5204E-07	Calculated			
103	concentration of chemical in sediment (g/kg dry)	Cs	3.2988E-04	Calculated			
104	concentration of chemical in sediment solids (g/kg dry)	Cssolids	3.2973E-04	Calculated	3.8186E-06		
105	concentration of chemical in sediment normalized with orga	Csorg	8.2470E-03	Calculated			
106	concentration of chemical in pore water (g/L)	Cwdp	1.8717E-07	Calculated			
107	concentration of chemical in phytoplankton (g/kg ww)	Cp	4.2890E-03	Calculated	1.4034E-05		
108	concentration of chemical in zooplankton (g/kg ww)	Cz	1.8868E-03	Calculated	6.1738E-06		
109	concentration of chemical in Benthos (g/kg ww)	Cb	1.6014E-03	Calculated	5.7195E-06		
110	concentration of chemical in forage fish A (g/kg ww)	Cffa	3.8112E-03	Calculated	1.2586E-05		
111	concentration of chemical in forage fish B (g/kg ww)	Cffb	5.2414E-03	Calculated	1.7308E-05		
112	concentration of chemical in piscivorous fish A (g/kg ww)	Cpfa	8.2507E-03	Calculated	2.7142E-05		
113	concentration of chemical in prey item for Zooplankton (g/kg PCDt)	PCDt	0.00428895	Calculated			
114	concentration of chemical in prey item for Benthos (g/kg PCDb)	PCDb	0.00032988	Calculated			
115	concentration of chemical in prey item for forage fish A (g/kg PCDffa)	PCDffa	0.00174407	Calculated			
116	concentration of chemical in prey item for forage fish B (g/kg PCDffb)	PCDffb	0.00174407	Calculated			
117	concentration of chemical in prey item for piscivorous fish A (g/kg PCDpfa)	PCDpfa	0.0045263	Calculated			
118							
119							
120	<b>BAF at steady-state</b>						
121		BAF	logBAF				
122	Benthos	2995.17119	3.47642165				
123	Forage Fish A	8892.546	3.83838597	Calculated			
124	Forage Fish B	9479.16094	3.9787699	Calculated			
125	Piscivorous Fish A	14921.5502	4.17381394	Calculated			
126	Note: the steady-state evaluation is based on constant chemical emission with the loading amount entered in cell "C43"						
127							

Food Web input values for the Bioaccumulation model are included in columns FWModel!G through FWModel!L.

The food web structure is included in rows 5 through 13. . The food web aquatic organism individual parameters are included in rows 18-38. The below page displays the recommended values for these rows:

	H	I	J	K	L	M	N	O	P	Q
4										
5	<b>Food Web Structure</b>									
6	Species	Phytoplankton	Zooplankton	Benthos	Forage Fish A	Forage Fish B	Piscivorous Fish A	Action		
7	Sediment	n/a	n/a	100%	n/a	n/a	n/a	Enter		
8	Phytoplankton	0%	100%	0%	n/a	n/a	n/a	Enter		
9	Zooplankton		0%	0%	50%	50%	0%	Enter		
10	Benthos			0%	50%	50%	0%	Enter		
11	Forage Fish A				0%	0%	50%	Enter		
12	Forage Fish B					0%	50%	Enter		
13	Piscivorous Fish A						0%	Enter		
14										
15										
16										
17										
18	<b>Aquatic Organisms Parameters</b>									
19	Definition	Units	Parameter	Phytoplankton	Zooplankton	Benthos	Forage Fish A	Forage Fish B	Piscivorous Fish A	Action
20	Weight of biota	kg	Wb	0.0000001	0.000001	0.01	0.01	1	Enter	
21	Lipid fraction in biota / (phytoplankton)	kg/kg	vlb	0.50%	2%	2%	4%	4%	Enter	
22	Nonlipid organic matter fraction in biota / (phytoplankton)	kg/kg	vnb	20.00%	20%	22%	22%	20%	Enter	
23	Water fraction in biota	kg/kg	wvb	79.50%	78.00%	74.00%	72.00%	76.00%	Enter	
24	Nonlipid organic matter-octanol proportionality constant	unitless	beta	0.35	0.035	0.035	0.035	0.035	Enter	
25	Dietary absorption efficiency of lipid	%	el	75%	72%	75%	92%	92%	Enter	
26	Dietary absorption efficiency of nonlipid organic matter	%	en	75%	72%	25%	55%	55%	Enter	
27	Dietary absorption efficiency of water	%	eww	25%	25%	25%	25%	25%	Enter	
28	fraction of the respiratory ventilation that involves overlying water	%	mo	95%	95%	95%	100%	100%	Enter	
29	fraction of the respiratory ventilation that involves sediment-associated	%	mp	5%	5%	5%	0%	0%	Enter	
30	Particle scavenging efficiency	%	sigma	100%	100.00%	100%	-----	-----	Enter	
31	resistance to chemical uptake through the aqueous		A	0.00006	-----	-----	-----	-----	Enter	
32	resistance to chemical uptake through the organic phase		B	5.5	-----	-----	-----	-----	Enter	
33	Invertebrate growth rate coefficient (T < 17.5 deg C)	unitless	lgr	0.000502	0.000502	0.000502	0.000502	0.000502	Enter	
34	Invertebrate growth rate coefficient (T > 17.5 deg C)	unitless	Fgr	0.00251	0.00251	0.00251	0.00251	0.00251	Enter	
35	Constant Aew	unitless	Aew	1.85	1.85	1.85	1.85	1.85	Enter	
36	Constant Bew	unitless	Bew	155	155	155	155	155	Enter	
37	Constant Aed	unitless	Aed	-----	0.0000003	0.0000003	0.0000003	0.0000003	Enter	
38	Constant Bed	unitless	Bed	-----	2	2	2	2	Enter	
39										

The calculated parameters for each aquatic organism in the food web are included in rows 40 through 77 and 79-89. The below pages display the recommended values for these rows:

	G	H	I	J	K	L	M	N	O	P	Q	R	S
40		<b>Calculated Parameters</b>											
41		Definition	Units	Parameter	Phytoplankton	Zooplankton	Benthos	Forage Fish A	Forage Fish B	Piscivorous Fish A			
42		volume of lipid in organism	kg	Vl	-----	2.00E-09	0.0000002	0.0004	0.0006	0.04	Calculated		
43		volume of NLOM in organism	kg	Vnlom	-----	2.00E-08	0.0000002	0.0022	0.0022	0.2	Calculated		
44		volume of water in organism	kg	Vw	-----	0.000000078	0.0000078	0.0074	0.0072	0.76	Calculated		
45		Gill uptake rate constant	L/kg day	k1	9644.312847	23777.46355	4744.227897	422.8297386	422.8297386	84.96562431	Calculated		
46		Dietary uptake rate constant	kg/kg day	kd	0	0.335929671	0.168336603	0.059737682	0.059737682	0.029939763	Calculated		
47		Gill elimination rate constant	/day	k2	1.021347316	6.963621322	1.395410907	0.0704034	0.04969681	0.014256496	Calculated		
48		Fecal egestion rate constant	/day	ke	-----	0.041853904	0.065495391	0.005953807	0.00419509	0.004757496	Calculated		
49		Growth dilution rate constant	/day	kg	0.1	0.01260967	0.00502	0.006304835	0.006304835	0.00251	Calculated		
50		Metabolic transformation rate constant	/day	km	0	0	0	0	0	0	Calculated		
51		total elimination rate constant	/day	kdtotal	1.121347316	7.040084896	1.465926298	0.082662041	0.060106608	0.021523952	Calculated		
52		time to reach 95% of steady-state	day	t95	2.675353084	0.42564754	2.046487606	36.28235317	49.91131953	139.3796103	Calculated		
53		kdike (max theoretical BLMF)	kg diet/kg pred BLMF			6.026244644	2.570616474	10.0352716	14.23950503	6.293190642	Calculated		
54		kdiktal	kg diet/kg pred BLMF			0.047662546	0.114951383	0.722673681	0.963962174	1.360697522	Calculated		
55													
56													
57													
58													
59													
60													
61		Biota-water partition coefficient	unitless	Kbw	-----	3399.88	3399.88	6005.81	8523.65	5917.71	Calculated		
62		Phytoplankton-water partition coefficient	unitless	Kpw	9442.7	-----	-----	-----	-----	-----	Calculated		
63		Gut-biota partition coefficient	unitless	Kgb	-----	0.160608534	0.516881923	0.147303944	0.103791291	0.244276569	Calculated		
64		Gill ventilation rate	L/day	Gv	-----	0.004401758	0.087826624	7.827556081	7.827556081	156.1802767	Calculated		
65		Feeding rate	kg/day	Gd	-----	6.84547E-08	3.43089E-06	0.001217315	0.001217315	0.061010285	Calculated		
66		Fecal egestion rate	kg/day	Gf	-----	4.47454E-08	2.57315E-06	0.000823635	0.000823635	0.03968719	Calculated		
67		Efficiency of chemical transfer via gill	%	Ew	54.02%	54.02%	54.02%	54.02%	54.02%	54.02%	Calculated		
68		Efficiency of chemical transfer via intestinal tract	%	Ed	-----	49.07%	49.07%	49.07%	49.07%	49.07%	Calculated		
69		Lipid fraction in diet	kg/kg	vid	-----	0.500%	0.00000%	2.00%	2.00%	5.0000%	Calculated		
70		Lipid fraction in gut	kg/kg	vlg	-----	0.002141819	0	0.002364785	0.002364785	0.006149116	Calculated		
71		Nonlipid organic matter fraction in diet	kg/kg	vnd	-----	20.000%	4.00000%	20.00%	20.00%	22.000%	Calculated		
72		Nonlipid organic matter fraction in gut	kg/kg	vng	-----	0.085672761	0.04	0.133018031	0.133018031	0.152190623	Calculated		
73		Water fraction in diet	kg/kg	vid	-----	79.500%	96.00000%	78.00%	78.00%	73.0000%	Calculated		
74		Water fraction in gut	kg/kg	vvg	-----	0.91218542	0.96	0.864617204	0.864617204	0.841660261	Calculated		
75		Water fraction in phytoplankton	kg/kg	vwp	-----	-----	-----	-----	-----	-----	Calculated		
76		Dissolved oxygen concentration	mg O2/L	Cox	8.964	8.964	8.964	8.964	8.964	8.964	Calculated		
77		Oxygen consumption	mg O2/day	Vox	-----	0.027620153	0.551094499	49.1163489	49.1163489	980	Calculated		

	G	H	I	J	K	L	M	N	O	P	Q	R	S
79		Concentration at steady-state	g/kg ww		0.004238951	0.001886765	0.001801368	0.003811208	0.005241391	0.008250697	Calculated		
80		BAF at steady-state	L/kg	BAF	7756.654023	3412.251612	2995.171193	6892.645996	9479.160943	14621.55016	Calculated		
81		BAF (freely dissolved) at steady-state	L/kg		8600.647196	3783.535036	3314.759391	7642.627386	17143251698	26985921181	Calculated		
82		BSAF at steady-state	kg OC/kg lipid	BSAF	-----	1.14E+01	9.71E+00	1.16E+01	1.06E+01	2.50E+01	Calculated		
83													
84													
85													
86		Lipid Equivalent Concentration in organism	g/kg eq lp	Cpredator	0.285809763	0.062879171	0.053367897	0.07472096	0.073816468	0.164994019	Calculated		
87		Lipid Equivalent Concentration in prey	g/kg eq lp	Cprey	0.285809763	0.008247025	0.058123534	0.058123534	0.058123534	0.07368922	Calculated		
88		BLMF	kg eq lipid/kg e BLMF		0.220003578	6.471169541	1.285554315	1.289992778	2.449184472	Calculated			
89		Organism-Water Fugacity Ratio at steady-state	unitless	BAF	0.220003578	6.471169541	1.285554315	1.289992778	2.449184472	Calculated			
90													
91													
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## Step 6 – Review the Foodweb tab

Go to the **Foodweb** tab. All values in this tab are automatically summarized from the **FWModel** tab. Thus, the user will never make any revisions to this tab.

The **Foodweb** tab summarizes the calculated k-values and the Feeding Matrix from the **FWModel** tab. The **Foodweb** tab is where the Bioaccumulation model actually reads in its input values to populate the foodweb and generate organism concentrations.

The page below displays a copy of the **Foodweb** tab with recommended calculated masses, lipid fractions, k-rates, and feeding matrix for the food web.

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## Step 7 – Confirm Run Parameters and Run Simulation

Go to the **AGRO** tab

The screenshot shows the CEMC Agrochemical Model interface. The 'Run' tab is active, displaying various input parameters and simulation results. The 'Run' button is highlighted. The 'Calculate Timestep' button is also visible. The 'Recalc timestep at start?' checkbox is checked. The 'Data Source: For normal Dynamic Mode check this' checkbox is checked. The 'uses GetPRZM-Files as data source' checkbox is checked. The 'Using data from GetPRZM-Files is recommended for Dynamic Runs' checkbox is checked. The 'Turn this option off to experiment with modified values in PRZM-forinput' checkbox is checked. The 'Outputs in new workbook (default)' checkbox is FALSE. The 'Outputs in this workbook' checkbox is FALSE. The 'Outputs in separate file' checkbox is TRUE. The 'Model start time' is 8/28/2007 13:47:01. The 'Model end time' is 8/28/2007 13:47:04. The 'Model run time' is 00:03:0. The 'Model Mass in' is 2.5912452136119700. The 'Model Mass Out' is 2.5897994705808500. The 'Model Storage (sed+water+pure)' is 0.0014995589624495. The 'Model total accounting' is 2.5912950295433000. The 'Model total accounting (%)' is 100.002%.

Parameter	Value
Model start time	8/28/2007 13:47:01
Model end time	8/28/2007 13:47:04
Model run time	00:03:0
Model Mass in	2.5912452136119700
Model Mass Out	2.5897994705808500
Model Storage (sed+water+pure)	0.0014995589624495
Model total accounting	2.5912950295433000
Model total accounting (%)	100.002%

Select either dynamic mode or steady-state mode. If Steady-state mode is selected then the emission scenario automatically changes to “Constant Inputs” as defined on the **Emissions** tab. When the dynamic mode is selected a message box appears to remind the user to select the appropriate emissions scenario as the PRZM-based scenario is NOT automatically selected when the model runs in dynamic mode.

The screenshot shows a dialog box titled "DYNAMIC EMISSION SCENARIO CHECK". The text inside the dialog box reads: "Please confirm that the type of dynamic emission scenario you wish to run is either: Constant Inputs or PRZM Inputs by checking cell "B12". Choose the appropriate Emission Scenario on the "Emissions" worksheet." There is an "OK" button at the bottom of the dialog box.

Enter the number of years of the simulation in cell AGRO!B14.

To output daily, enter “24” in cell AGRO!B15.

Use the “calculate timestep” button to fill in the appropriate timestep for the modelled system in cell AGRO!B16.

Select the “Outputs in separate file” option.

Cell AGRO!P2 will read 1 if steady-state mode is selected or 2 if dynamic mode is selected.

Cell AGRO!P3 should be set to “TRUE” so that the Bioaccumulation model is run in addition to the QWASI water quality model.

Also, cell AGRO!P4 should also be set to “True” so the timestep set as constant for the entire simulation, otherwise the model attempts to recalculate the timestep required at each iteration.

Examine cells AGRO!B4 – AGRO!B8 to make sure that the correct chemical, environmental scenario, foodweb, and dynamic simulation model options are selected.

Click the “Run AGRO” button to run the simulation.

To monitor the progress of a simulation, each simulation day number is displayed on the lower left-hand corner as it is being processed.

Upon completion of a simulation, Cells AGRO!B24 – AGRO!B33 display the model run time and simulation mass balance.

## Step 8 – Examine the output from the simulation

The output from the dynamic mode simulation is displayed in tabs **DYN-results-pond**, **DYN-timeseries**, and **DYN-yearly**. The output from the steady-state mode simulation is displayed in the tab named **SS-results-pond**. An overview of the format of the dynamic results is presented, followed by an overview of the steady-state results.

### Dynamic Results

The results presented in the **DYN-results-pond** tab are in the same format as the QWASI model with the foodweb results output at the bottom. These results reflect the **conditions at the end of the simulation**.

The following series of pages display an example of output contained in the **DYN-results-pond** tab.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	<b>CHEM Agrochemical Model</b>																			
2	Version 1.16.05 - BETA version																			
3																				
4	Simulation ID		Updated Foodweb calcs from Aug3 Gobas model																	
5	Additional Comments		BETA version - mods by LKR@CEIC																	
6	Date: 28/08/2007		Time: 13:47:04																	
7																				
8	Chemical:		testazole																	
9	Environment:		Modeling for EFED Report																	
10	Total Simulation Time:																			
11																				
12	<b>CHEMICAL PARAMETERS</b>																			
13																				
14	<b>Physical Properties</b>																			
15																				
16	Chemical Type		1																	
17	Molar Mass		345.6 g/mol																	
18	Temperature		17 °C																	
19																				
20	Log Kow		5.1																	
21	Solubility		1.79 g/m³																	
22	Vapour Pressure		1.2399E-08 Pa																	
23	Melting Point		125 °C																	
24	Fugacity Ratio		0.075981																	
25	Sub-cooled Liquid V.P.		1.5524E-07 Pa																	
26	Henry's Law Constant		2.3939E-06 Pa m³/mol																	
27																				
28	<b>Partition Coefficients</b>																			
29																				
30	Air-Water (Kaw)		Dimensionless L/kg																	
31	Suspended Particles-Water		9.9236E-10 -																	
32	Sediment-Water		8299.84345 3458.268106																	
33	Resuspended Particles-Water		4955.13042 2084.637675																	
34	Aerosol-Air		4955.13042 2084.637675																	
35	Organic Carbon-Water (Koc)		3.8649E+13 -																	
36																				
37	Half-lives																			
38			Half-life																	
39			Rate Constant																	
40	Water		1/h																	
41	Sediment		240 0.002888113																	
42			960 0.000722028																	

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	
44	ENVIRONMENT PARAMETERS																						
45	Lake Data																						
46																							
47																							
48																							
49																							
50	Water	Area	Depth	Volume																			
51	Sediment	10000	m	m³																			
52		10000		2																			
53				0.01																			
54		Inflow	Outflow																				
55	Water	m³/h	m³/h																				
56	Suspended Particles	4.16668E-06	5	5																			
57				0.0000625																			
58	Sediment Subcompartment Volumes																						
59	Solids	50																					
60	Pore-Water	50																					
61																							
62																							
63	Particle Properties																						
64																							
65		Density	Conc. of	Volume	OC																		
66		kg/m³	Particles	Fraction	Fraction																		
67	Particles in Water Column	2400	30 mg/L	0.0000125	0.067																		
68	Sediment Solids	2400		0.5	0.04																		
69	Inflow Particles	2400	2 mg/L	8.33333E-07	0.067																		
70	Resuspended Particles	2400			0.04																		
71	Aerosols in Air	9500	30 µg/m³	2E-11	0																		
72																							
73																							
74	Transfer Rates																						
75																							
76	Mass Transfer Coefficients	m/h																					
77	Volatilization (air side)	1																					
78	Volatilization (water side)	0.01																					
79	Sediment-water Diffusion	0.0004																					
80	Aerosol Dry Deposition Velo.	10																					
81																							
82	Aerosol Scavenging Ratio	200000																					
83																							
84																							
85																							
86	Rain Rate	0	1 m/year	Aerosol Depo. m³/h																			
87	Sediment Deposition Rate	0.000690556	50 g/m²/day	Vet	0																		
88	Sediment Resuspension Rat.	0.000394444	40 g/m²/day	Dry	0.000002																		
89	Sediment Burial Rate	0.00173611	10 g/m²/day	Total	0.000002																		
90																							
91																							
92																							
93																							
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98																							
99																							
100																							

[illegible]

## DYN-results-pond tab, Rows 92 - 228, continued.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
177														
178	<b>Rate Details</b>													
179														
180		kg/year	mol/h											
181	Emission to Water	0	0											
182	Water Inflow	0	0											
183	Particle Inflow	0	0											
184														
185	Rain Dissolution	0	0											
186	Aerosol Deposition - Wet	0	0											
187	Aerosol Deposition - Dry	0	0											
188														
189	Absorption	0	0											
190	Volatilization	2.5427E-09	8.39864E-13											
191														
192	Sediment Deposition	0.01846006	6.09755E-06											
193	Sediment Resuspension	0.0293109	9.68169E-06											
194														
195	Water to Sediment Diffusion	0.00102489	3.3853E-07											
196	Sediment to Water Diffusion	0.00340719	1.12543E-06											
197														
198	Water Transformation	0.01633522	5.39569E-06											
199	Sediment Transformation	0.1524065	5.03414E-05											
200														
201	Sediment Burial	0.00732772	2.42042E-06											
202														
203	Water Outflow	0.00128111	4.23163E-07											
204	Particle Outflow	0.00013291	4.39023E-08											
205														
206														
207	<b>D Values &amp; Response Times</b>													
208														
209		D Value	Response Time					Response Time						
210			of Water					of Sediment						
211		mol/Pa.h	years	days	hours			years	days	hours				
212	Burial	3593591.82	0	0	0	0	3.28833472	1200.24217	28805.81216					
213	Sediment Transformation	74741721.8	0	0	0	0	0.15810357	57.7078016	1384.987239					
214	Sediment Resuspension	14374367.3	0.073231566	26.72952151	641.5085163	0.82208368	300.060543	7201.453039						
215	Water to Sediment Diffusion	1670921.82	0.629986041	229.9449048	5518.677716	7.07210391	2581.31793	61951.63026						
216	Sediment Deposition	30096331.5	0.03497627	12.76633863	306.3921272	0.39263698	143.312498	3439.499959						
217	Water Transformation	28632098.2	0.039525892	14.42695041	346.2468098	0	0	0						
218	Volatilization	4.14540877	253933.3229	92685662.85	2224455908	0	0	0						
219	Volat. (air side)	4.14540918												
220	Volat. (water side)	41773045.6												
221	Water Outflow	2088652.28	0.503988833	183.9559239	4414.942173									
222	Water Particle Outflow	216693.587	4.857815309	1773.102588	42554.46211									
223	Rain Dissolution	0	11415525.11	4166666667	1E+11									
224	Wet Particle Deposition	0	11415525.11	4166666667	1E+11									
225	Dry Particle Deposition	32043.3024	32.85109036	11990.64798	287775.5516									
226	Water Inflow	2088652.28	0.503988833	183.9559239	4414.942173									
227	Water Particle Inflow	14446.2271	72.86729036	26596.56098	638317.4636									
228														
229														

**DYN-results-pond** tab, Rows 229 - 250 display echoes of the input for the Food Web aquatic organism masses, lip fraction, k-rates and feeding table matrix used by the Bioaccumulation model.

	A	B	C	D	E	F	G	H	I	J	K
230	FOODWEB RESULTS										
231											
232	Foodweb Characteristics										
233	Organism	Mass (kg)	Lipid Fraction	k1	k2	ke	kd	km		kg	kT
234	Phytoplankton	0	0.005	9644.312647	1.021347316		0	0		0	0 1
235	Zooplankton	0.0000001	0.02	23777.46355	6.993621322	0.041853904	0.33592967			0	0 7
236	Benthic Invertebrates	0.00001	0.02	4744.227697	1.395410907	0.065495391	0.16836366			0	0 1
237	Forage Fish A	0.01	0.04	422.8297386	0.0704034	0.005953807	0.05973768			0	0 0
238	Forage Fish B	0.01	0.06	422.8297386	0.049606681	0.00419509	0.05973768			0	0 0
239	Piscivorous Fish	1	0.04	84.36562431	0.014256466	0.004757486	0.02993976			0	0 0
240											
241	Feeding Table										
242		Phytoplankton	Zooplankton	Benthic Invertebrates	Forage Fish A	Forage Fish B	Piscivorous Fish				
243	Water, dissolved	0	0	0	0	0	0				
244	Sediment, particles	1	0	0	0	0	0				
245	Phytoplankton	0	0	1	0	0	0				
246	Zooplankton	0	1	0	0	0	0				
247	Benthic Invertebrates	0	0	0	0.5	0.5	0				
248	Forage Fish A	0	0	0	0.5	0.5	0				
249	Forage Fish B	0	0	0	0	0	0.5				
250	Piscivorous Fish	0	0	0	0	0	0.5				

**DYN-results-pond** tab, Rows 251 - 263 display calculated results of pesticide concentrations from the Bioaccumulation model for each aquatic organism in the food web. The organism Biomagnification Factors (BMFs) and the Theoretical Maximum BMFs (calculated by kd/ke) are presented.

Type a question for help											
Arial 10 B I U											
A278											
	A	B	C	D	E	F	G	H	I	J	K
251	FOODWEB Results										
252											
253	Concentrations										
254		ug/kg	g/kg		BMF	Theoretical Max BMF, kd/ke					
255											
256	Water, dissolved	0.029249033	2.9249E-08								
257	Sediment, particles	200.7595832	0.00020076								
258	Phytoplankton	285.0027664	0.000285003								
259	Zooplankton	123.7998954	0.0001238		0.047662546	8.026244644					
260	Benthic Invertebrates	130.1200778	0.00013012		0.114851383	2.570618474					
261	Forage Fish A	316.1773736	0.000316177		0.722673681	10.03352716					
262	Forage Fish B	492.7512153	0.000492751		0.993862174	14.23990503					
263	Piscivorous Fish	6632.415719	0.006632416		1.390997522	6.293190642					
264											
265											
266											
267											
268											
269											
270											
271											
272											
273											
274											
275											
276											
277											
278											
AGRO / Chemical / Environment / GetPRZM_Files / Emissions / Foodweb / FWMModel / DYH-results-pond / DYH-tmeseries / DYH-yearly / SS-results-pond / PRZM-forInput / PRZM											

The **DYN-timeseries** tab contains the values of selected output variables for each day of the simulation.

An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!P** is displayed below. These columns summarize the daily simulation date, emission, fugacities for each bulk media, and bulk media chemical concentrations in natural units.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Time (h)	Year	Month	Day	Emission kg/year	Fugacity, Pa				Bulk Concentrations (natural units)						
2						Water	Sediment	Inflow	Air				Water, ng/L	Sediment, ng/m3	Inflow, ng/L	Air, ug/m3
3	0	1961	5	12	0	0	0	0	0	0	0	0	0	0	0	0
4	24	1961	5	13	0	1.3E-10	4.83385E-13	3.707E-10	0	0	0	20306.92813	172932040.5	71616.50282	0	0
5	48	1961	5	14	0	1.1E-10	1.35508E-12	0	0	0	0	17922.30308	484784687.3	0	0	0
6	72	1961	5	15	0	9.6E-11	2.09168E-12	0	0	0	0	15289.41262	748303193.9	0	0	0
7	96	1961	5	16	0	8.2E-11	2.6999E-12	0	0	0	0	13049.06468	965897203.9	0	0	0
8	120	1961	5	17	0	7E-11	3.1993E-12	0	0	0	0	11142.62027	1144556663	0	0	0
9	144	1961	5	18	0	6E-11	3.60647E-12	0	0	0	0	9520.202258	1290224549	0	0	0
10	168	1961	5	19	182.5	7.1E-11	3.9355E-12	0	0	0	0	11264.38615	1407953362	0	0	0
11	192	1961	5	20	0	1.9E-10	4.8154E-12	0	0	0	0	29842.88113	1722739580	0	0	0
12	216	1961	5	21	0	1.6E-10	5.98684E-12	0	0	0	0	25474.53025	2141805650	0	0	0
13	240	1961	5	22	0	1.4E-10	6.94633E-12	0	0	0	0	21757.15283	2485067301	0	0	0
14	264	1961	5	23	0	1.2E-10	7.72632E-12	0	0	0	0	18593.5109	2764108682	0	0	0
15	288	1961	5	24	0	1E-10	8.5432E-12	0	0	0	0	15900.89572	2988777956	0	0	0
16	312	1961	5	25	0	8.5E-11	8.85374E-12	0	0	0	0	13608.95676	3167446801	0	0	0
17	336	1961	5	26	182.5	1.1E-10	9.24447E-12	5.26211E-10	0	0	0	16771.90322	3307231133	254081.866	0	0
18	360	1961	5	27	0	2.9E-10	1.05366E-11	4.94791E-10	0	0	0	46946.14905	3769507763	164049.663	0	0
19	384	1961	5	28	0	2.7E-10	1.23803E-11	4.16959E-10	0	0	0	42979.92547	4429091717	108676.5174	0	0
20	408	1961	5	29	0	2.4E-10	1.39769E-11	1.6158E-10	0	0	0	37866.30352	5000259500	25011.56927	0	0
21	432	1961	5	30	0	2E-10	1.52963E-11	0	0	0	0	32482.18771	5472294134	0	0	0
22	456	1961	5	31	0	1.7E-10	1.63547E-11	0	0	0	0	27789.35146	5850918657	0	0	0
23	480	1961	6	1	0	1.5E-10	1.71897E-11	0	0	0	0	23794.613	6149649959	0	0	0
24	504	1961	6	2	182.5	1.5E-10	1.7836E-11	0	0	0	0	23518.71931	6380880634	0	0	0
25	528	1961	6	3	0	2.5E-10	1.894E-11	0	0	0	0	40376.78899	6775843983	0	0	0
26	552	1961	6	4	0	2.7E-10	2.02572E-11	0	0	0	0	34542.93204	7247060994	0	0	0

An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!D** and then window split to display columns **DYN-timeseries!R - DYN-timeseries!Z** is displayed below. These columns summarize the daily chemical concentrations for aquatic organism in the food web.

	A	B	C	D	Q	R	S	T	U	V	W	X	Y	Z
1	Time (h)	Year	Month	Day	Foodweb Concentrations, ng/g									
2					Water-dissolved only, ug/L	Sediment-solids only	Phytoplankton	Zooplankton	Benthic Invertebrates	Forage Fish A	Forage Fish B	Piscivorous Fish		
3	0	1961	5	12	0	0	0	0	0	0	0	0	0	0
4	24	1961	5	13	18.3983639	144.0809566	78164.026	62030.63277	35014.77677	6133.13	6173.2782	1045.09162		
5	48	1961	5	14	16.2378599	403.9057268	120730.5011	57853.61079	48710.55016	15653.4	15920.994	2770.38887		
6	72	1961	5	15	13.8524239	623.4601737	120012.5353	50344.87764	45645.77312	23411.4	24086.13	4529.8241		
7	96	1961	5	16	11.822637	804.7519288	107526.3843	43278.37173	39801.94883	29311.7	30521.786	6281.82178		
8	120	1961	5	17	10.0953714	953.6047714	93352.90391	37063.51999	34187.51531	33624.6	35452.438	8003.56073		
9	144	1961	5	18	8.62543778	1074.970183	80230.63547	31714.04962	29281.80141	36629.6	39120.521	9676.38235		
10	168	1961	5	19	10.205693	1173.057733	71987.98925	35137.18164	26675.75931	38721.1	41891.534	11315.8057		
11	192	1961	5	20	27.038072	1435.326652	152532.9679	93506.25142	63046.36948	47362.8	51264.594	14135.0053		
12	216	1961	5	21	23.0802844	1784.477914	185511.8276	83122.19457	72569.92899	58259.2	63083.711	17518.9007		
13	240	1961	5	22	19.7122879	2070.471574	175000.4979	71974.19784	65764.42861	66493.8	72400.716	20831.8332		
14	264	1961	5	23	16.8459836	2302.959139	154528.7067	61832.62265	57018.28398	72273.9	79356.182	24044.9195		
15	288	1961	5	24	14.4064362	2490.145758	133660.5589	53004.93264	48987.85019	76005.2	84300.292	27132.017		
16	312	1961	5	25	12.3299071	2639.00642	114868.1109	45431.66969	42034.92367	78074.6	87576.734	30073.0551		
17	336	1961	5	26	15.1955813	2755.46986	103868.6877	52049.11296	38701.78198	79059.6	89730.105	32902.6031		
18	360	1961	5	27	42.5338745	3140.622656	235288.035	146759.0701	97859.66961	90918.1	102787.3	37580.7892		
19	384	1961	5	28	38.9404199	3690.165048	301279.5108	139552.5357	118842.1362	107564	120901.93	43273.4452		
20	408	1961	5	29	34.3074061	4166.042163	296263.1154	124823.7845	112323.3712	120998	136055.62	48969.7209		
21	432	1961	5	30	29.4293211	4559.32499	267006.4187	107893.5729	99106.75061	130635	147569.74	54516.7726		
22	456	1961	5	31	25.1775451	4874.781763	232734.7769	92627.09826	85579.76433	136799	155678.36	59835.0704		
23	480	1961	6	1	21.5582556	5123.674285	200606.8726	79461.94202	73552.68943	140104	160919.68	64888.0964		
24	504	1961	6	2	21.3082921	5316.327635	175613.9479	76196.64357	64804.72924	141267	163955.8	69681.969		

An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!D** and then window split to display columns **DYN-timeseries!AA - DYN-timeseries!AJ** is displayed below. These columns display the daily concentrations in the dissolved water column, benthic sediment and pore water along with the total daily input of chemical mass, total daily output of chemical mass, daily water inflow rate, daily water outflow rate, and net daily water volume flux.

	A	B	C	D	AA	AB	AC	AD	AE	AF	AH	AI	AJ
1	Time (h)	Year	Month	Day	Water-dissolved only-ug/L-2	Sediment solids only ng/g	Conc porewater ug/L		SumInput, kg	SumLoss, kg	Water inflow m3/h	Water outflow m3/h	Net water m3/h
2													
3	0	1961	5	12	0	0	0		0	0	5	5	0
4	24	1961	5	13	18.39836386	0.144080957	0.069785105		0.439666399	0.439666465	10.08333	10.08333	0
5	48	1961	5	14	16.23785987	0.403905727	0.195630319		0.454831194	0.454831721	5	5	0
6	72	1961	5	15	13.8524239	0.623460174	0.301970743		0.454831194	0.454831721	5	5	0
7	96	1961	5	16	11.82263701	0.804751929	0.389778768		0.454831194	0.454831721	5	5	0
8	120	1961	5	17	10.09537143	0.953604771	0.461875119		0.454831194	0.454831721	5	5	0
9	144	1961	5	18	8.625437785	1.074970183	0.520658029		0.454831194	0.454831721	5	5	0
10	168	1961	5	19	10.20569304	1.173057733	0.568166389		0.517331194	0.517331721	5	5	0
11	192	1961	5	20	27.03807204	1.435326652	0.695195418		0.954831194	0.954831721	5	5	0
12	216	1961	5	21	23.08028441	1.784477914	0.864305605		0.954831194	0.954831721	5	5	0
13	240	1961	5	22	19.71228793	2.070471574	1.002825628		0.954831194	0.954831721	5	5	0
14	264	1961	5	23	16.84598363	2.302959139	1.115430163		0.954831194	0.954831721	5	5	0
15	288	1961	5	24	14.40643623	2.490145758	1.206093344		0.954831194	0.954831721	5	5	0
16	312	1961	5	25	12.32990715	2.63900642	1.278193482		0.954831194	0.954831721	5	5	0
17	336	1961	5	26	15.19558134	2.75546986	1.33460214		1.058873579	1.058877616	54.5	54.5	0
18	360	1961	5	27	42.53387448	3.140622656	1.521149543		1.797845806	1.797875133	21.69167	21.69167	0
19	384	1961	5	28	38.94041986	3.690165048	1.787318469		1.87718513	1.877219789	14.14167	14.14167	0
20	408	1961	5	29	34.30740611	4.166042163	2.017807876		1.909914237	1.909950634	6.0625	6.0625	0
21	432	1961	5	30	29.4293211	4.55932499	2.208293031		1.913098522	1.913134945	5	5	0
22	456	1961	5	31	25.17754514	4.874781763	2.36108341		1.913098522	1.913134945	5	5	0
23	480	1961	6	1	21.55825564	5.123674285	2.481633628		1.913098522	1.913134945	5	5	0
24	504	1961	6	2	21.30829206	5.316327635	2.574944601		1.975598522	1.975634945	5	5	0



An example of output contained in columns **DYN-timeseries!A - DYN-timeseries!D** and then window split to display columns **DYN-timeseries!AL - DYN-timeseries!AX** is displayed below. These columns display the particle solid fluxes in the water column and benthic sediment along with various water and sediment daily fluxes in mol basis.

	A	B	C	D	AL	AM	AN	AO	AP	AQ	AR	AS	AT	AU	AV	AW	AX
1	Time (h)	Year	Month	Day	Sed Inflow m3/h	Sed Resusp m3/h	Sed outflow m3/h	Sed Dep m3/h	Net Sed m3/h		timestep.h	d_inv_V/mol	Inv_V/mol	d_inv_S/mol	Inv_S/mol		Inv_Pure/mol
2																	
3	0	1961	5	12	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	0	0	0	0	0	0
4	24	1961	5	13	0.000410521	0.008944444	0.000126042	0.008680556	-0.001451232	0	3	-0.018191747	1.175169452	0.012229953	0.050038206	0	0
5	48	1961	5	14	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.020834582	1.037170317	0.010579719	0.140273347	0	0
6	72	1961	5	15	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.017727788	0.864603971	0.008759367	0.216522915	0	0
7	96	1961	5	16	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.015085105	0.755154206	0.007215691	0.279454145	0	0
8	120	1961	5	17	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.012837186	0.644827582	0.005907257	0.33117959	0	0
9	144	1961	5	18	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.010925043	0.550937631	0.004798824	0.373328663	0	0
10	168	1961	5	19	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	0.1715464	0.851874198	0.003860419	0.407393913	0	0
11	192	1961	5	20	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.03458616	1.727018584	0.016880867	0.468477688	0	0
12	216	1961	5	21	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.029414053	1.4742205	0.013882896	0.618725431	0	0
13	240	1961	5	22	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.025031535	1.259094492	0.011335629	0.719058926	0	0
14	264	1961	5	23	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.021303633	1.076013362	0.009178214	0.799799966	0	0
15	288	1961	5	24	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.018132534	0.920190725	0.007382208	0.864808436	0	0
16	312	1961	5	25	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.015435043	0.787555368	0.005807914	0.916506598	0	0
17	336	1961	5	26	0.015387385	0.008944444	0.00069125	0.008680556	0.012680024	0	3	0.282811468	0.970596251	0.004503065	0.956953453	0	0
18	360	1961	5	27	0.003389054	0.008944444	0.000271146	0.008680556	0.001381797	0	3	-0.029731371	2.716791033	0.02547157	1.090714052	0	0
19	384	1961	5	28	0.001372436	0.008944444	0.000176771	0.008680556	-0.000540446	0	3	-0.039438499	2.487264205	0.022670049	1.28156589	0	0
20	408	1961	5	29	5.276E-05	0.008944444	7.57813E-05	0.008680556	-0.001759132	0	3	-0.042492527	2.191337009	0.01918162	1.446834346	0	0
21	432	1961	5	30	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.037128102	1.879756233	0.015523356	1.583418442	0	0
22	456	1961	5	31	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.031603312	1.608180061	0.012350224	1.692974148	0	0
23	480	1961	6	1	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.026903269	1.377030367	0.009668677	1.779412604	0	0
24	504	1961	6	2	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	0.157939647	1.361036997	0.007404119	1.846319628	0	0
25	528	1961	6	3	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.048155507	2.336819733	0.019316059	1.960603004	0	0
26	552	1961	6	4	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.036207102	1.999012271	0.015372177	2.06050519	0	0
27	576	1961	6	5	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.033444463	1.711627212	0.012038226	2.204565707	0	0
28	600	1961	6	6	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.028474324	1.468664397	0.009222665	2.287879359	0	0
29	624	1961	6	7	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.024246321	1.258644301	0.008847639	2.350706979	0	0
30	648	1961	6	8	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.020646571	1.061240584	0.004846935	2.39525885	0	0
31	672	1961	6	9	0.010051693	0.008944444	0.000544323	0.008680556	0.007691259	0	3	0.033139065	0.980366484	0.00316424	2.427270155	0	0
32	696	1961	6	10	4.33876E-06	0.008944444	6.2787E-05	0.008680556	-0.001794559	0	3	-0.022340408	1.168028363	0.005578557	2.463823059	0	0
33	720	1961	6	11	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.019054415	1.004534551	0.003750887	2.500019031	0	0
34	744	1961	6	12	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.016233345	0.865959268	0.002213726	2.52293205	0	0
35	768	1961	6	13	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.013633499	0.740279294	0.000923263	2.534693729	0	0
36	792	1961	6	14	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.011791662	0.645015965	-0.00015195	2.537120063	0	0
37	816	1961	6	15	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.01005436	0.558584289	-0.001049923	2.531756296	0	0
38	840	1961	6	16	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.008576315	0.485056825	-0.001795771	2.519808786	0	0
39	864	1961	6	17	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.007318592	0.42223935	-0.002412576	2.502689134	0	0
40	888	1961	6	18	4.16696E-06	0.008944444	0.0000625	0.008680556	-0.001794444	0	3	-0.006246341	0.368622041	-0.002919962	2.451039288	0	0

The following table summarizes the columns in the columns of the **DYN-timeseries tab**:

**Table 6: Summary of timeseries output parameters included with the model**

Variable/Parameter	Description (if necessary)
Time (h)	
Year	From PRZM3.12
Month	From PRZM3.12
Day	From PRZM3.12
Emission kg/year	(if it occurs at this output interval)
<b>Fugacity, Pa</b>	
Water	
Sediment	
Inflow	
Air	
Pure Phase Chemical	
<b>Bulk Concentrations (natural units)</b>	
Water, ng/L	
Sediment, ng/m <sup>3</sup>	
Inflow, ng/L	
Air, ug/m <sup>3</sup>	
<b>Foodweb Concentrations, ng/g</b>	
Water-dissolved only, ug/L	
Sediment-solids only	
Phytoplankton	
Zooplankton	
Benthic Invertebrates	
Forage Fish A	
Forage Fish B	
Piscivorous Fish	
<b>Other</b>	
SumInput kg	Cumulative system Input of chemical
SumLoss kg	Cumulative system Loss of chemical
Water inflow m <sup>3</sup> /h	
Water outflow m <sup>3</sup> /h	
Net water m <sup>3</sup> /h	Inflow-Outflow
Sed Inflow m <sup>3</sup> /h	
Sed Resusp m <sup>3</sup> /h	
Sed outflow m <sup>3</sup> /h	
Sed Dep m <sup>3</sup> /h	
Net Sed m <sup>3</sup> /h	Inflow + Resusp – Outflow – Dep

The **DYN-yearly** tab contains the Estimated Environmental Concentrations (EECs) for the peak, 4-day, 21-day, 60-day, 90-day and Annual running averages for the chemical dissolved water column (for the highest 4 years of the simulation), benthic sediment sorbed chemical (for the highest 4 years of the simulation), and chemical dissolved in benthic pore water (for all years).

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	Summary of Annual Peak Values - units are ppb - ug/L, ug/kg, and ug/L																
2	Water																
3	Year	Peak	4day	21day	60day	90day	Annual										
4	1961	42.53387451	36.30275345	24.35691643	12.49514771	8.525496483	2.154887676										
5	1962	31.01566124	24.93386078	19.93797112	11.02113247	7.522340298	1.902371883										
6	1963	31.01575089	25.44404221	20.14524078	10.72341728	7.318989277	1.85038209										
7	1964	42.71648788	40.13788986	30.72669411	16.53958702	11.281847	2.839358091										
8	Sediment	30.99331665	27.12480927	22.31699371	14.01089096	9.574266434	2.425187826										
9	Year	Peak	4day	21day	60day	90day	Annual										
10	1967	31.47005272	29.92352676	21.74877548	12.22539043	8.339946747	2.108692646										
11	1968	72.00937653	59.31645966	40.47285461	18.68839645	12.72089481	3.19989419										
12	1969	33.16246033	29.44874763	23.94294739	13.3897562	9.12955761	2.307548285										
13	1970	42.79794312	35.40646744	28.73192437	14.7636652	10.0782671	2.549487591										
14	Pore-water	36.5101738	29.27306557	24.50738507	13.74801922	9.399575233	2.377716303										
15	Year	Peak	4day	21day	60day	90day	Annual										
16	1973	51.16928864	41.02540588	27.44241142	15.242342	10.4207468	2.637946844										
17	1974	32.97999954	26.53116989	21.17629814	11.24765491	7.683871746	1.943422794										
18	1975	44.74221039	36.68009567	26.93260765	14.24290848	9.721645355	2.458840132										
19	1976	56.2098465	46.97554398	32.39645386	15.9214344	10.86883926	2.739059687										
20	1977	90.52404785	76.41593933	40.25551987	18.97348595	12.9533186	3.272400856										
21	1978	57.40812683	46.25005722	27.95661354	15.41656113	10.54681301	2.671898918										
22	1979	33.71849823	27.07398605	21.93412209	14.25864697	9.78395462	2.477102518										
23	1980	58.22719193	46.70570755	32.38362122	16.56999779	11.33562374	2.858613253										
24	1981	46.2473526	38.83179092	28.05111313	14.63220787	9.999668121	2.526949883										
25	1982	51.69116211	42.57536697	30.68570709	14.87016392	10.1333828	2.560456799										
26	1983	46.56212997	40.17373657	27.60877991	14.2075367	9.6854496	2.447705746										
27	1984	46.14097214	42.36930084	31.020895	15.72977829	10.74557114	2.709403038										
28	1985	40.90264511	32.82274246	24.83531189	12.7513876	8.761656761	2.217543602										
29	1986	30.98724174	24.91360474	20.51253891	12.08961105	8.243132591	2.085828304										
30	1987	31.25631714	25.13958168	21.07585144	12.66717243	8.728728294	2.209665537										
31	1988	48.05846405	40.38293076	30.06317139	15.91494083	10.85391903	2.735218048										
32	1989	30.9382782	24.92571449	19.96682739	11.05440617	7.610530376	1.928925633										
33	1990	61.74824142	50.65732574	32.09967804	15.67603207	10.6972456	2.702696323										
AGRO / Chemical / Environment / GetPRZM_Files / Emissions / Foodweb / FWMModel / DYN-results-pond / DYN-timeseries / DYN-yearly / SS-results-pond / PRZM-forInput / PRZM																	
40	1985	3.481950998	3.474330187	3.306331873	2.759078264	2.332169056	0.74858433										
41	1986	3.265149117	3.258912802	3.135131121	2.592978477	2.188745499	0.702758729										
42	1987	3.235586166	3.228167534	3.078638315	2.670116901	2.289322615	0.742867887										
43	1988	4.564675808	4.55505085	4.333664281	3.477374792	2.8973279	0.91848278										
44	1989	2.936492682	2.930020094	2.788197756	2.360131502	2.009531975	0.652857423										
45	1990	4.476986885	4.468397617	4.254661083	3.457499266	2.871734619	0.90665102										

## Steady-state Results

The results presented in the **SS-results-pond** tab are in the same format as the QWASI model with the foodweb results output at the bottom.

The following series of pages display an example of output contained in the **SS-results-pond** tab.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	<b>CEMC SFU Agrochemical Model</b>																
2	<b>Version 12</b>																
3																	
4	Simulation ID		Enter simulation name														
5	Additional Comments		Enter user name or additional information														
6	Date: 18/09/2007		Time: 10:35:51 AM														
7																	
8	Chemical:		Test Chemical														
9	Environment:		Modeling for EFED Report														
10																	
11																	
12	<b>CHEMICAL PARAMETERS</b>																
13																	
14	<b>Physical Properties</b>																
15																	
16	Chemical Type		1														
17	Molar Mass		345.6 g/mol														
18	Temperature		17 °C 290.15 K														
19																	
20	Log Kow		5.1														
21	Solubility		179 g/m³ 0.005173398 mol/m³														
22	Vapour Pressure		1.2398E-08 Pa														
23	Melting Point		125 °C 398.15 K														
24	Fugacity Ratio		0.07986781														
25	Sub-cooled Liquid V.P.		1.5524E-07 Pa														
26	Henry's Law Constant		2.3939E-06 Pa m³/mol														
27																	
28	<b>Partition Coefficients</b>																
29			Dimensionless: L/kg														
30	Air-Water (Kaw)		9.3236E-10														
31	Suspended Particles-Water		8239.84345 3458.269106														
32	Sediment-Water		4955.13042 2064.637675														
33	Resuspended Particles-Water		4955.13042 2064.637675														
34	Aerosol-Air		3.8649E+13														
35	Organic Carbon-Water (Koc)		- 51615.94188														
36																	
37	Half-lives																
38																	
39																	
40	Water		240		0.002888113												
41	Sediment		960		0.000722028												
42																	
43																	
44	<b>ENVIRONMENT PARAMETERS</b>																
45																	

[illegible]

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
92	<b>RESULTS</b>																
93																	
94	Chemical Input																
95		to Air	to Water	to Sediment													
96	Emission, kg/yr	0	0.05604	0													
97	Chemical Concentration in Inflow W	0	ng/L														
98	Chemical Concentration in Air	0	ng/m³														
99																	
100	fZ = C																
101		Fugacity	Z Values	Concentrations													
102		Pa	mol/m³Pa	kg/m³	mol/m³												
103	<b>Bulk Air</b>	0	0.320847565	0	0	0	ng/m³										
104	Air vapour		0.000414541	0													
105	Aerosols		160263523	0													
106	<b>Bulk Water</b>	3.3471E-13	461983.9515	5.33333E-08	1.54321E-07	53.3332546	ng/L										
107	Water Solution		417730.4558	4.83207E-08	1.39817E-07												
108	Water Particles		3467097389	0.000401054	0.00160457	167.105875	ng/g										
109	Pure Phase Chemical	N/A															
110	<b>Bulk Inflow</b>	0	4.20619.3555	0	0	0	ng/L										
111	Inflow Water			0													
112	Inflow Particles		3467097389	0	0												
113	<b>Bulk Sediment</b>	1.1266E-13	1035163310	4.03035E-05	0.00016619	40303495.1	ng/m³										
114	Sediment Pore Water			1.62641E-08	4.70605E-08	16.2640979	ng/L										
115	Sediment Solids		2063908889	8.05907E-05	0.000233191	33.5794632	ng/g										
116	Resuspended Solids		2063908889														
117	Rain	0		0	0	0	ng/L										
118																	
119	<b>Amounts</b>																
120																	
121	Amount						Amount Sorbed										
122		mol	kg	%			(% of amount in bulk phase)										
123	Bulk Water	0.00308642	0.001066665	20.32725206			%										
124	Water Solution	0.0027963	0.000968402	18.9601491				Water									
125	Water Particles	0.00029011	0.000100264	1.967102957				Sediment									
126	Bulk Sediment	0.0186189	0.00403035	79.07274794				Inflow									
127	Sediment Pore Water	2.353E-06	8.13205E-07	0.05545531				Air									
128	Sediment Solids	0.0185954	0.004029536	79.05679341													
129	Pure Phase Chemical	0	0	0													
130	System Total	0.01474831	<b>0.00509701</b>	100													
131	<b>Mass Balances</b>																
132																	
133																	
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
134	<b>In the System</b>																
135	Total Chemical Inputs			kg/yr	mol/h												
136	Emission			0.05604	1.8												

# SS-results-pond tab, Rows 92 - 228, continued.

	Name Box	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
178	Rate Details																	
179																		
180			kg/gear	mol/h														
181	Emission to Water		0.05604	1.85106E-05														
182	Water Inflow		0	0														
183	Particle Inflow		0	0														
184																		
185	Rain Dissolution		0	0														
186	Aerosol Deposition - Wet		0	0														
187	Aerosol Deposition - Dry		0	0														
188																		
189	Absorption		0	0														
190	Volatilization		4.2006E-09	1.38749E-12														
191																		
192	Sediment Deposition		0.03049682	1.00734E-05														
193	Sediment Resuspension		0.0049026	1.61938E-06														
194																		
195	Water to Sediment Diffusion		0.00169316	5.59267E-07														
196	Sediment to Water Diffusion		0.00056989	1.88242E-07														
197																		
198	Water Transformation		0.02698649	8.9192E-06														
199	Sediment Transformation		0.02549183	8.42022E-06														
200																		
201	Sediment Burial		0.00122565	4.04845E-07														
202																		
203	Water Outflow		0.00211645	6.99084E-07														
204	Particle Outflow		0.00021958	7.25286E-08														
205																		
206																		

207	D Values & Response Times																	
208																		
209		D Value	Response Time of Water			Response Time of Sediment												
210																		
211		mol/Pa.h	years	days	hours	years	days	hours										
212	Burial	359359182	0	0	0	3.28833472	1200.24217	28806										
213	Sediment Transformation	747417218	0	0	0	0.15810357	57.7078016	1385										
214	Sediment Resuspension	14374367.3	0.073231566	26.72952151	6415085163	0.82208368	300.060543	72015										
215	Water to Sediment Diffusion	167092182	0.629986041	229.9449048	5518.677716	7.07210391	2581.31733	61952										
216	Sediment Deposition	300963315	0.03497627	12.76633963	306.3921272	0.39263698	143.312498	3439.5										
217	Water Transformation	26632098.2	0.039525892	14.42695041	346.2468098	0	0	0										
218	Volatilization	4.14540877	253933.3229	92685662.85	2224455908	0	0	0										
219	Volat. (air side)	4.14540918																
220	Volat. (water side)	41773045.6																
221	Water Outflow	208852.28	0.503988833	183.9559239	4414.942173													
222	Water Particle Outflow	216693.587	4.857815309	1773.102588	42554.46211													
223	Rain Dissolution	476861251	2.207471086	805.7269465	19337.44672													
224	Wet Particle Deposition	73158.2247	14.38877758	5251.903816	126045.6916													
225	Dry Particle Deposition	32043.3024	32.85109036	11990.64798	287775.5516													
226	Water Inflow	208852.28	0.503988833	183.9559239	4414.942173													
227	Water Particle Inflow	14446.2391	72.86722964	26596.53882	638316.9317													
228																		

**SS-results-pond** tab, Rows 230 - 250 display echoes of the input for the Food Web aquatic organism masses, lip fraction, k-rates and feeding table matrix used by the Bioaccumulation model.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
230	FOODWEB RESULTS																
231																	
232	Foodweb Characteristics																
233	Organism	Mass (kg)	Lipid Fraction	k1	k2	ke	kd	km	kg	kT							
234	Phytoplankton	0	0.005	9644.312647	1.021347316	0	0	0	0.1	1.1213473							
235	Zooplankton	0.0000001	0.02	23777.46355	6.993621322	0.0418539	0.33592967	0	0.0126097	7.0480849							
236	Benthic Invertebrates	0.00001	0.02	4744.227697	1.395410907	0.06549539	0.16836366	0	0.00602	1.4659263							
237	Forage Fish A	0.01	0.04	422.8297386	0.0704034	0.00595381	0.05973768	0	0.0063048	0.082662							
238	Forage Fish B	0.01	0.06	422.8297386	0.049606681	0.00419509	0.05973768	0	0.0063048	0.0601066							
239	Piscivorous Fish	1	0.04	84.36562431	0.014256466	0.00475749	0.02993976	0	0.00251	0.021524							
240																	
241	Feeding Table																
242		Phytoplankton	Zooplankton	Benthic Invertebrates	Forage Fish A	Forage Fish B	Piscivorous Fish										
243	Water, dissolved	1	0	0	0	0	0										
244	Sediment, particles	0	0	1	0	0	0										
245	Phytoplankton	0	1	0	0	0	0										
246	Zooplankton	0	0	0	0.5	0.5	0										
247	Benthic Invertebrates	0	0	0	0.5	0.5	0										
248	Forage Fish A	0	0	0	0	0	0.5										
249	Forage Fish B	0	0	0	0	0	0.5										
250	Piscivorous Fish	0	0	0	0	0	0										

**SS-results-pond** tab, Rows 251 - 263 display calculated results of pesticide concentrations from the Bioaccumulation model for each aquatic organism in the food web. Bioconcentration Factors (BCFs), Biomagnification Factors (BMFs) and Bioaccumulation Factors (BAFs) are presented here.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
251																	
252	FOODWEB Results																
253																	
254	Concentrations																
255		ug/kg	g/kg	BCF	BMF	BAF to dissolved water											
256	Water, dissolved	0.04832068	4.83207E-08														
257	Sediment, particles	33.5794692	3.35795E-05														
258	Phytoplankton	401.803773	0.000401804	8600.647196	0	8600.6472											
259	Zooplankton	176.758634	0.000176759	3373.606292	0.047662546	3783.53504											
260	Benthic Invertebrates	155.051244	0.000155051	3236.334394	0.114851383	3318.88631											
261	Forage Fish A	367.063255	0.000367063	5115.162068	0.722673681	7596.40047											
262	Forage Fish B	504.806379	0.000504806	7034.663397	0.933862174	10447.0043											
263	Piscivorous Fish	795.782767	0.000795793	3919.615947	1.390997522	16468.7816											
264																	
265																	

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